Description of collective motions based on the dynamical GCM with the Gogny force

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Theoretical motivation

What is a GCM?
How should we restrict the GCM?
What can the restricted GCM do?

What is GCM ?

A standard explanation

1. Prepare wave functions parametrized with a generator coordinate *x*
2. Consider the superposition of these wave functions (path)
3. Solve the Hill-Wheeler equation

■ Generator Coordinate Method (GCM) D. L. Hill and J. A. Wheeler, Phys. Rev., **89**, 1102 (1953).

$$|\Psi\rangle_{\mathrm{GCM}} = \int dx\, f(x)|x\rangle$$

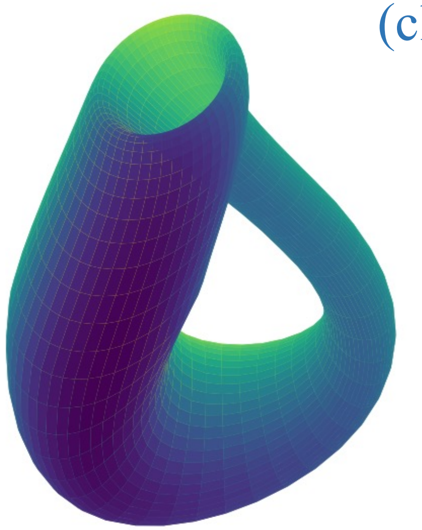
■ Hill-Wheeler equation

$$\int dx \left\{ \langle x'|\hat{H}|x\rangle - E\langle x'|x\rangle \right\} f(x) = 0$$

What is done in GCM?

■ Generator Coordinate Method (GCM)

input

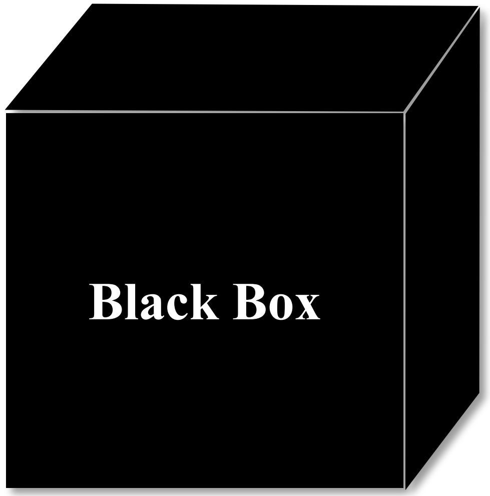


e.g., Klein bottle

(closed) linear span

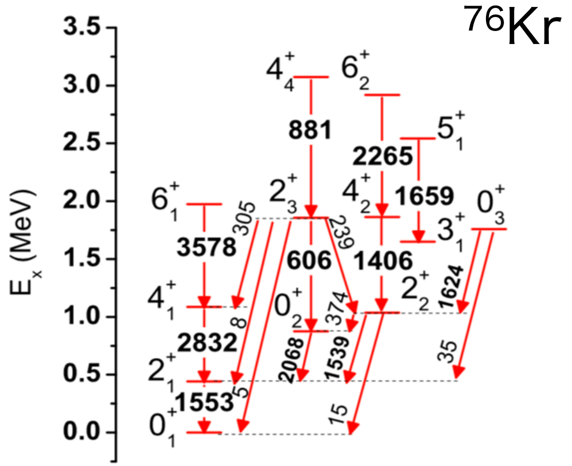
: $\overline{\text{Span}}$

collective subspace



projection & diagonalization

output



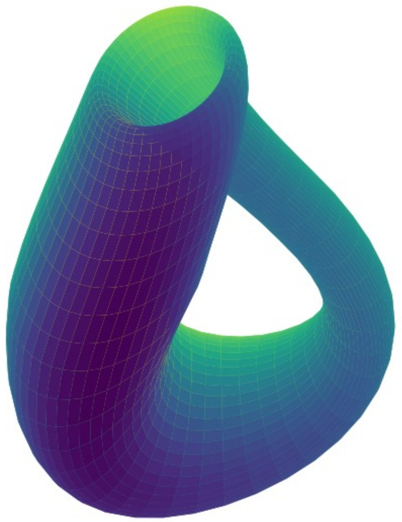
J. M. Yao *et al.*, Phys. Rev. C **89**, 054306 (2014).

1. Prepare the path (manifold) $|x\rangle$ as input, which is often generated empirically.
2. Generate the collective subspace with the (closed) linear span of the path.
3. Obtain eigenfunctions, eigenenergies, and etc…

What should we do in GCM?

■ Essential degree of freedom

input

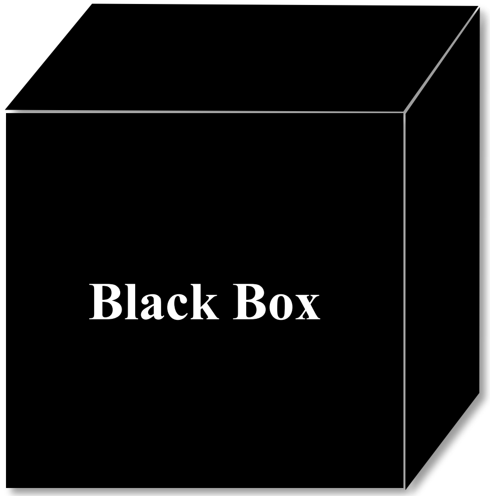


e.g., Klein bottle

uniquely determined

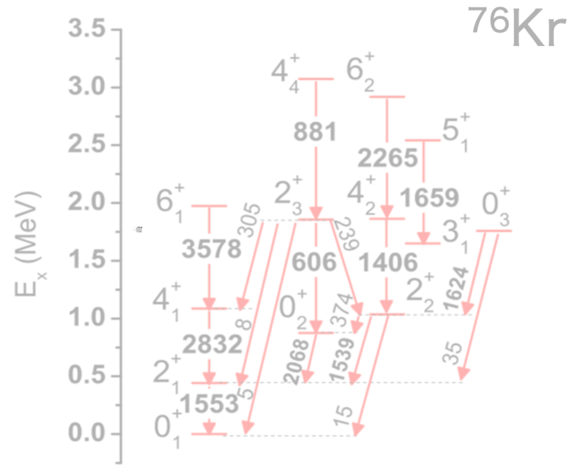
not uniquely determined

collective subspace



projection & diagonalization

output



J. M. Yao *et al.*, Phys. Rev. C **89**, 054306 (2014).

Essential degree of freedom is the collective subspace

Control the collective subspace with constraints on the path

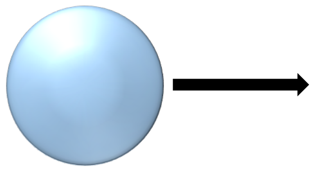
However, the mapping from the path to the collective subspace is extremely complex

What is necessary for the GCM is not an extension but a restriction

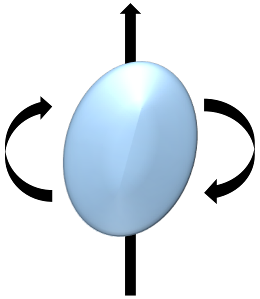
Description of collective motions

The GCM is often used in microscopic descriptions of collective motions

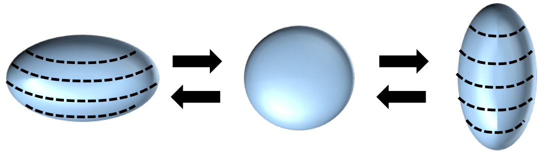
translational motion



rotational motion



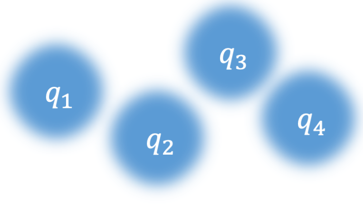
shape vibration



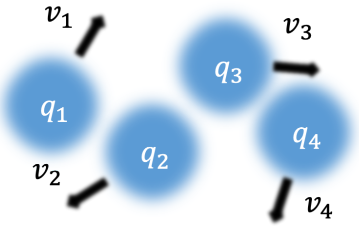
$\beta < 0\,,\quad \beta = 0,\quad \beta > 0$

- ✓ An empirical method often do not work well
- ✓ The double projection method solves this problem for collective motions associated with symmetries R.E. Peierls and D.J. Thouless, Nucl. Phys. **31**, 211 (1962).
- ■ What is an appropriate restriction on the description of the general collective motion?

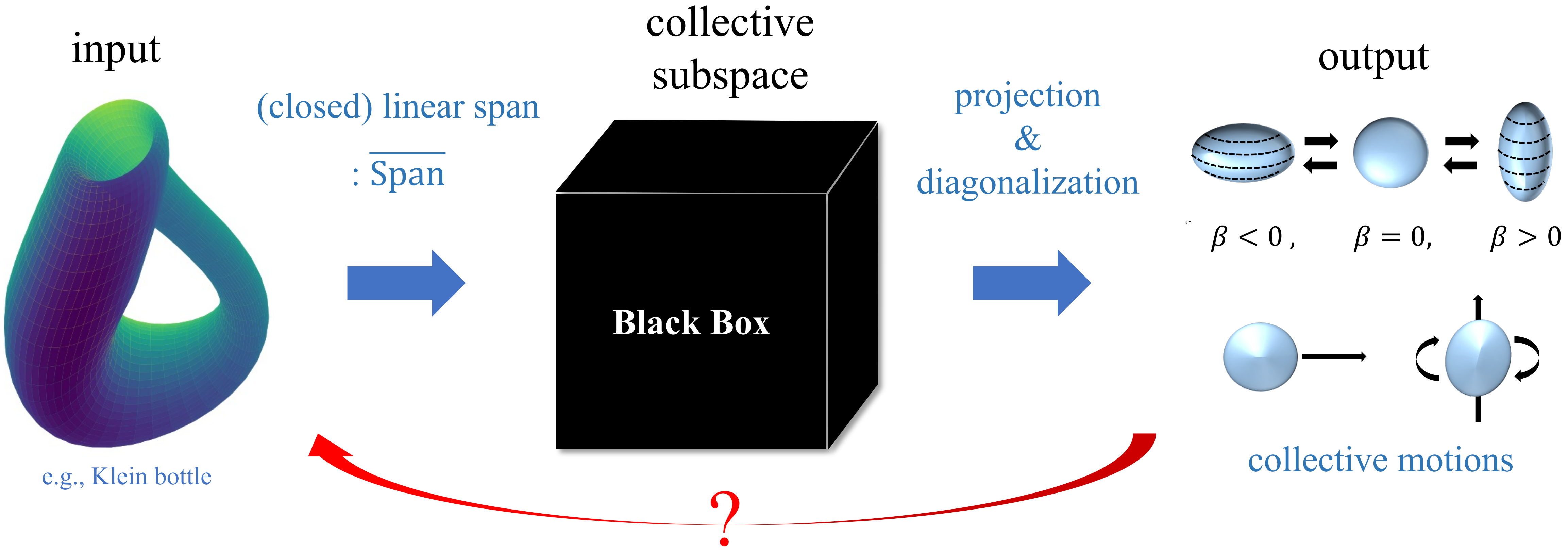
empirical



double projection



How to limit path?



We have decided what we want to describe with the GCM
However, the collective motion is not a rigorously defined object in general

What restrictions should be imposed on the path (manifold)?

Structures

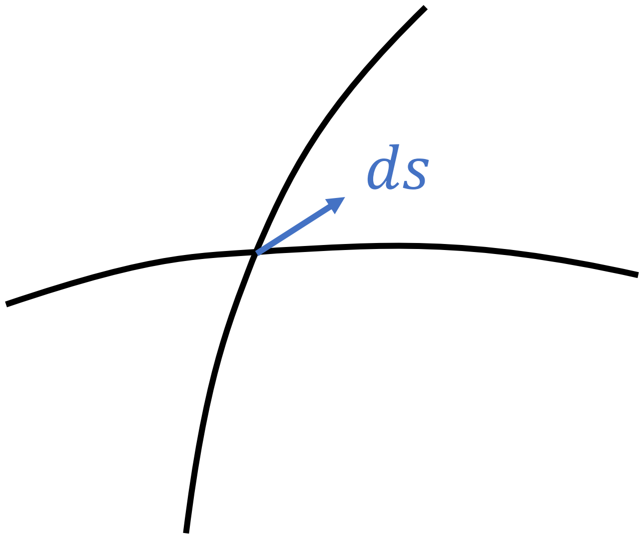
■ "Structures" in the manifold

e.g., distance

✓ Riemannian structure

✓ symplectic structure

✓ etc…

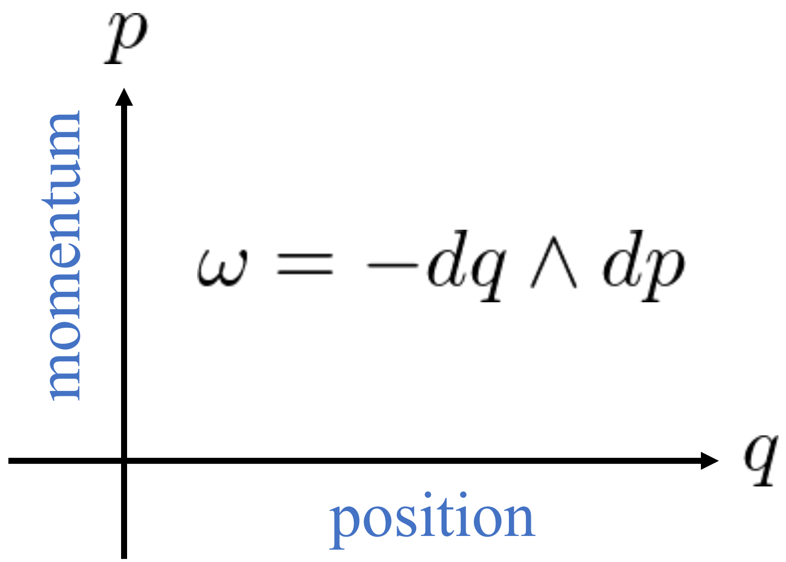


$$ds^2 = g_{\mu\nu}(x)dx^\mu dx^\nu$$

Structures

■ "Structures" in the manifold

e.g., analytical mechanics



- ✓ Riemannian structure
- ✓ symplectic structure
- ✓ etc…

What structure should we consider?

➡ Symplectic structure seems good for collective motions

Berry curvature

Quantum states have some “natural” structures

■ Fubini-Study metric

$$g_{\mu\nu} = \frac{1}{2}\langle x|\overleftarrow{\partial_\mu}\overrightarrow{\partial_\nu} + \overleftarrow{\partial_\nu}\overrightarrow{\partial_\mu}|x\rangle - \langle x|\overleftarrow{\partial_\mu}|x\rangle\langle x|\overrightarrow{\partial_\nu}|x\rangle$$

■ Berry curvature

$$B = i\langle x|\overleftarrow{\partial_\mu}\overrightarrow{\partial_\nu} - \overleftarrow{\partial_\nu}\overrightarrow{\partial_\mu}|x\rangle dx^\mu \wedge dx^\nu$$

If the dimension of x is even, B becomes symplectic structure

Berry curvature seems to be useful !

(They are unified with a quantum geometric tensor : J. P. Provost and G. Vallee, Commun. Math. Phys., 76, 289 (1980).)

Dynamical GCM

■ Dynamical GCM (DGCM)

K. Goeke and P.-G Reinhard, Ann. Phys. 124, 249 (1980).

➡ GCM with the symplectic structure in analytical mechanics

two-dimensional case (for simplicity)

$$(x^1, x^2) \to (q, p) \qquad |\psi\rangle_{\mathrm{DGCM}} = \iint dq dp\, f(q,p)|q,p\rangle$$

✓ symplectic form

$$B = -dq \wedge dp$$

$\Leftrightarrow$

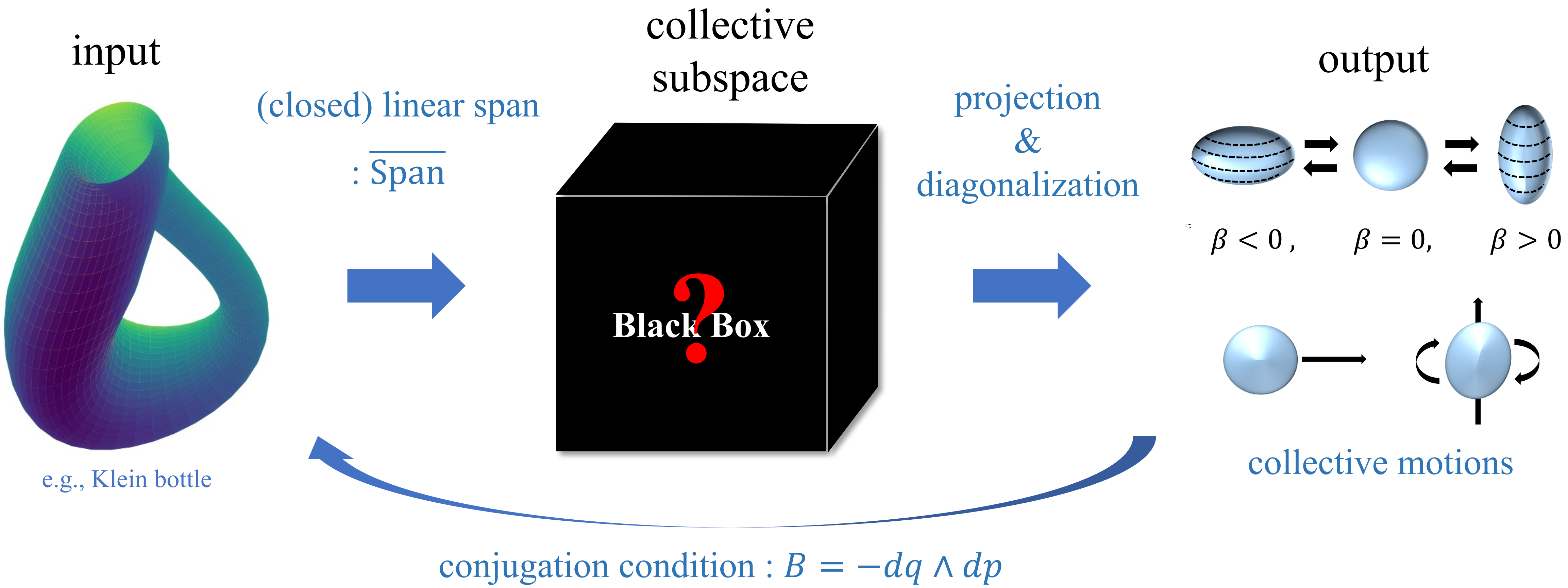
✓ conjugation condition

$$\langle q,p|\overleftarrow{\partial}_q \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_q|q,p\rangle = i$$

In this sense, p is the conjugate momentum of the coordinate q

(The DGCM includes the double projection method)

What is done in DGCM?



What structure does the DGCM's collective subspace has?

Structure of collective subspace

N. Hizawa, arXiv:2205.13058 (2022).

Information about collective degrees of freedom must be given externally

■ Collective operator $\hat{Q} = \hat{Q}_C \otimes \hat{\mathbf{1}}_{NC}$

$\hat{Q}_C : \mathcal{H}_C \to \mathcal{H}_C$ non-degenerated Hermitian operator

$\hat{\mathbf{1}}_{NC} : \mathcal{H}_{NC} \to \mathcal{H}_{NC}$ identity operator

Quantum mechanics is defined on $\mathcal{H}_C \otimes \mathcal{H}_{NC}$

■ Boundary condition

$$\langle q|\hat{Q}|q\rangle = q + \text{const.} \quad \to \quad |q,p\rangle := e^{i\hat{Q}p}|q\rangle$$

The path satisfies the conjugation condition $B = -dq \wedge dp$

($|q\rangle$ is not determined uniequly, but the rough structure is determined)

Constrained variational method + DGCM

■ Constrained variational method + DGCM

$$\delta\langle\psi|\hat{H}-\lambda(\hat{Q}-q)|\psi\rangle=0 \quad \rightarrow \quad |\psi\rangle=|q\rangle$$

$$\Rightarrow \quad \overline{\mathrm{Span}}(\{|q,p\rangle\}_{q,p})=\mathcal{H}_C\otimes\mathcal{H}_{NC}^{\mathrm{sub}}, \quad \mathcal{H}_{NC}^{\mathrm{sub}}\subseteq\mathcal{H}_{NC}$$

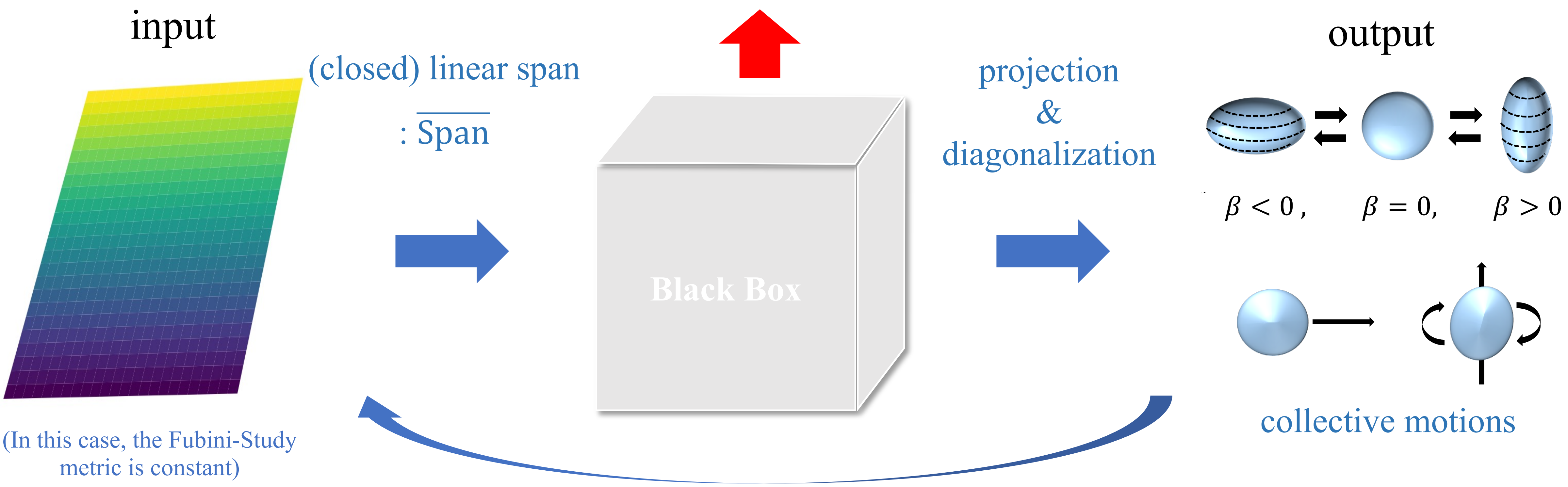
The collective subspace has the simple separable structure!

Then, several conditions are needed

- ✓ The collective motion is vibrational
- ✓ Interaction between the collective part and the others is negligible
- ✓ etc…

What is done in constrained variational method + DGCM?

$$\overline{\mathrm{Span}}(\{|q,p\rangle\}_{q,p}) = \mathcal{H}_C \otimes \mathcal{H}_{NC}^{\mathrm{sub}}$$



conjugation condition : $B = -dq \wedge dp$
(+ several conditions)

We can see what we are doing!

Constrained variational method + DGCM

■ Summary so far

- ✓ Essential degrees of freedom in the GCM is the collective subspace
- ✓ DGCM is a GCM with the symplectic structure in analytical mechanics
- ✓ Constrained variational method + DGCM yields the separable collective subspace for the vibrational motion (+ several conditions)

Numerical application

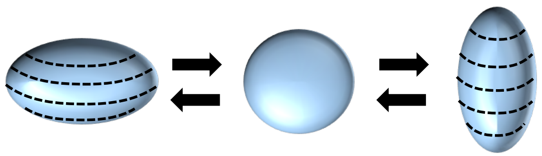
Quadrupole vibration of ^{16}O
What differences appear when introducing momentum?
Can we see the separable structure?

Numerical application

N. Hizawa, K. Hagino, and K. Yoshida, in press [arXiv:2204.01995 [nucl-th]]

- **Collective motion**

quadrupole vibration



$\beta < 0\,,\qquad \beta = 0,\qquad \beta > 0$

- **Collective operator**

$$\hat{\beta} = \frac{\sqrt{20\pi}}{3r_0^2 A^{5/3}} \int d^3r\, r^2 Y_{20}(\theta,\phi) \sum_{\sigma,\tau} \hat{\psi}^\dagger(\boldsymbol{r},\sigma,\tau)\hat{\psi}(\boldsymbol{r},\sigma,\tau)$$

$r_0 = 1.2$ fm

A : mass number

- **Collective coordinates**

$$\delta\langle \hat{H} - \lambda(\hat{\beta} - \beta)\rangle = 0 \quad \rightarrow \quad |\beta\rangle \quad \rightarrow \quad |\beta, p_\beta\rangle = e^{i\hat{\beta}p_\beta}|\beta\rangle$$

constrained variational method — usual GCM basis — dynamical path

Numerical detail

■ Numerical details

effective interaction	Gogny D1S [1] (exact Coulomb and CoM correction)
trial wave function	Hartree Fock (3D, no pairing)
single-particle basis	3D harmonic oscillator basis (up to $10\hbar\omega$)
nuclide	^{16}O
conventional GCM	$\lvert\psi\rangle_{\mathrm{GCM}} = \int d\beta\, f(\beta)\lvert\beta\rangle$
DGCM	$\lvert\psi\rangle_{\mathrm{DGCM}} = \iint d\beta dp_\beta\, f(\beta, p_\beta)\lvert\beta, p_\beta\rangle$

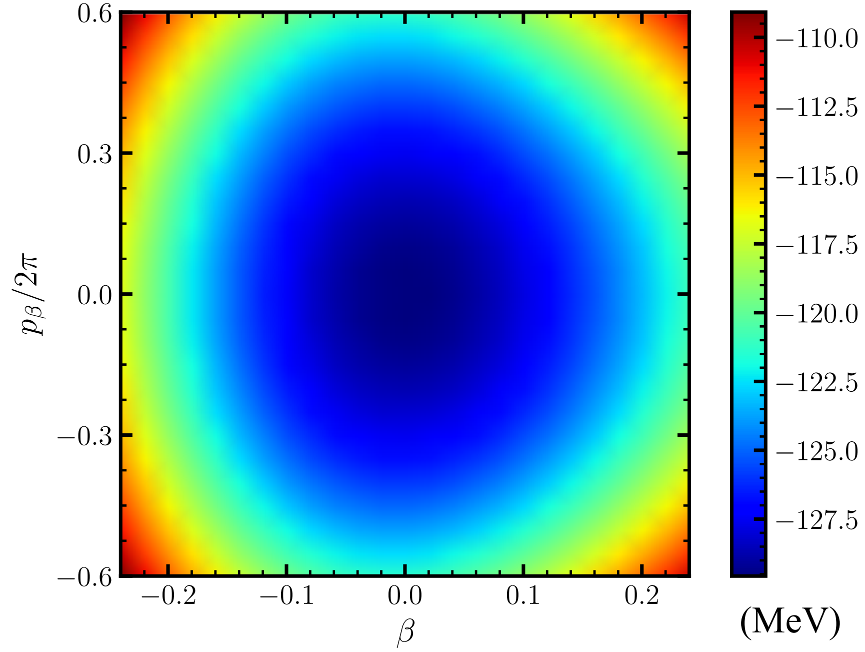
[1] J.F. Berger, M. Girod and D. Gogny, Comput. Phys. Commun. **63**, 365 (1991).

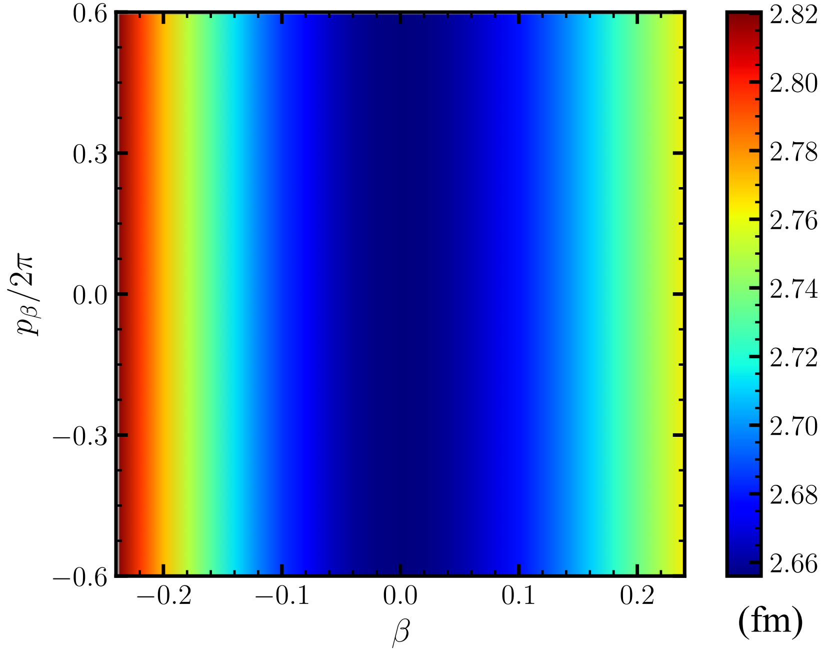
Dynamical path

- Energy surface and mean square radius

$$E(\beta, p_\beta) = \langle \beta, p_\beta | \hat{H} | \beta, p_\beta \rangle$$

$$r_{\mathrm{ms}}(\beta, p_\beta) = \left(\langle \beta, p_\beta | \sum_{i=1}^{A} \hat{\boldsymbol{r}}_i^2 | \beta, p_\beta \rangle / A \right)^{1/2}$$





✓ $\beta = -0.24, -0.22, \cdots, 0.24$ $\quad p_\beta/2\pi = -0.6, -0.55, \cdots, 0.6$ (total : 625 points)

✓ Symmetric with respect to the p_β-axis due to the time reversal symmetry

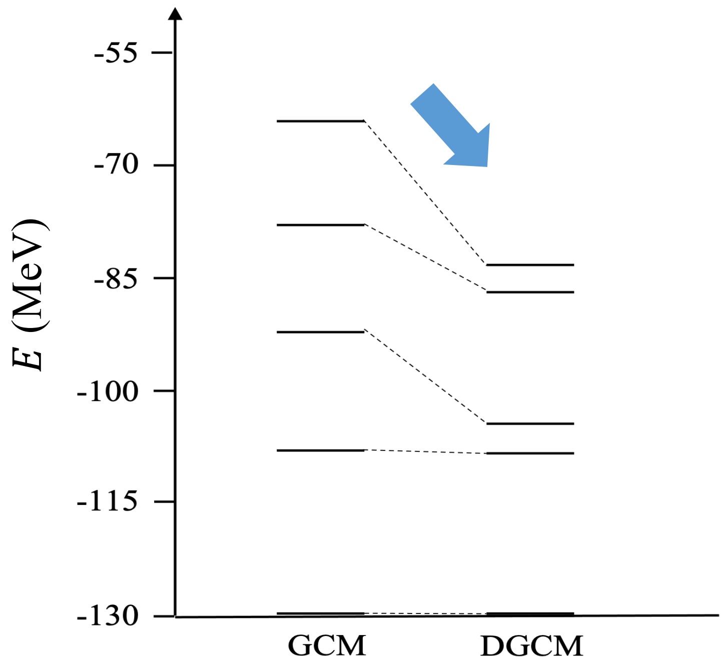
✓ The effect of internal excitations

GCM vs DGCM (energies)

- GCM vs DGCM (energies)

✓ GCM : $\beta = -0.24, -0.22, \cdots, 0.24 \quad p_\beta/2\pi = 0$ (25 points)

✓ DGCM : $\beta = -0.2, -0.1, \cdots, 0.2 \quad p_\beta/2\pi = -0.6, -0.3 \cdots, 0.6$ (25 points)



GCM and DGCM energy

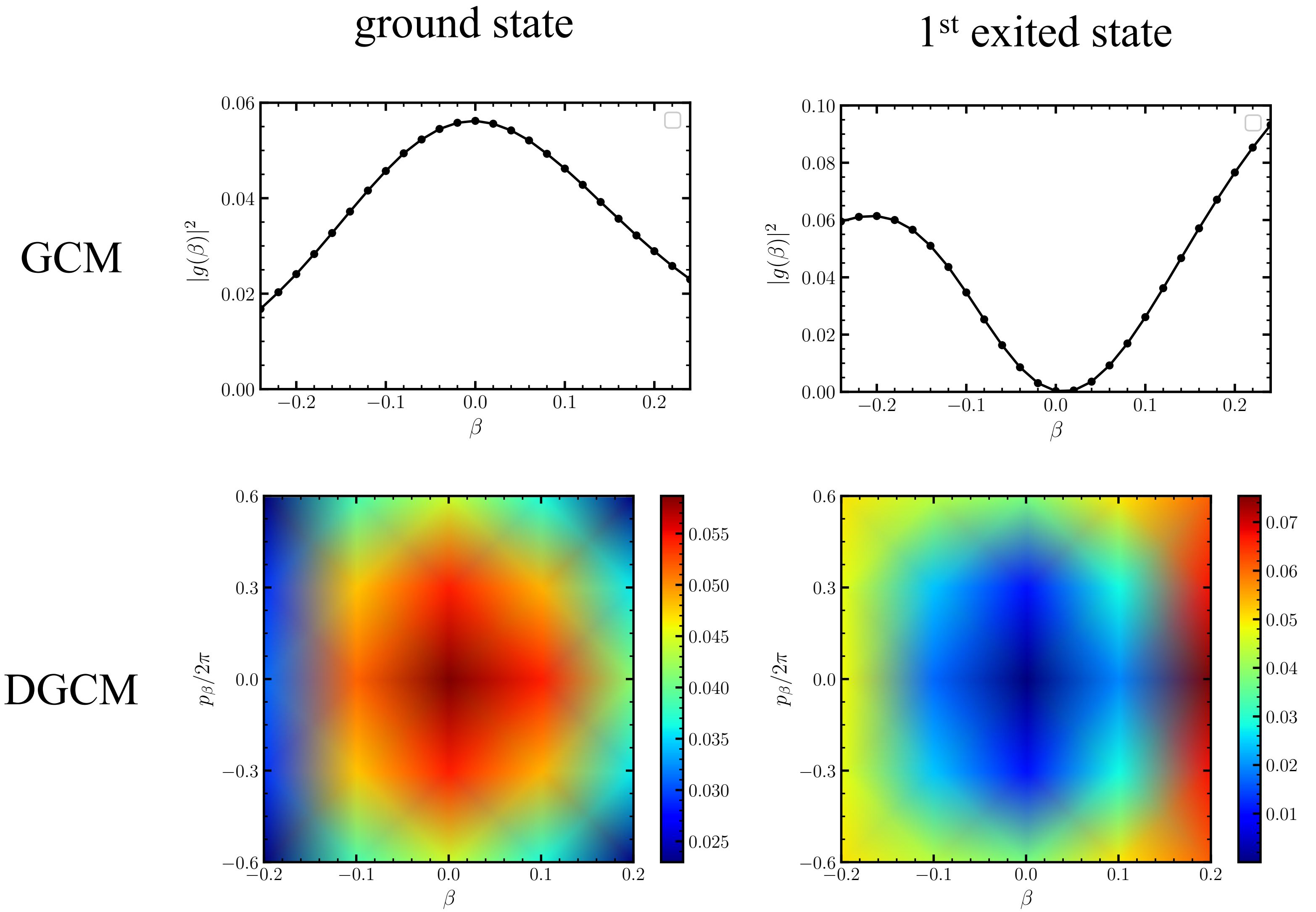
state	GCM (MeV)	DGCM (MeV)
GS	-129.682	-129.765
1st	-107.993	-108.140
2nd	-92.260	-104.475
3rd	-77.911	-87.019
4th	-64.097	-83.059

$$\min_{\beta, p_\beta} E(\beta, p_\beta) = E(0,0) = -129.569\,\mathrm{MeV}$$

✓ DGCM can generate different states more efficiently

Collective wave function (^{16}O)

- Collective wave function $|g(\beta)|^2$, $|g(\beta, p_\beta)|^2$



✓ In the DGCM, the wave functions also spread in the momentum direction

✓ The collective wave functions behave like a harmonic oscillator

Sum rule (GCM)

- Sum rule for the GCM

H. Flocard, D. Vautherin, Nucl. Phys. A **264**. 197 (1976).

$$\langle i|\hat{H}|j\rangle = E_i\langle i|j\rangle = E_i\delta_{ij}, \quad i \in \mathcal{X} \qquad (\hat{H}|i\rangle \neq E_i|i\rangle)$$

projection onto collective subspace ($= \overline{\mathrm{Span}}(\{|i\rangle \,|\, i \in \mathcal{X}\})$)

$$\hat{\pi} := \sum_{i\in\mathcal{X}} |i\rangle\langle i| \neq \hat{\mathbf{1}}_{\mathrm{tot}}$$

For any Hermitian operator $\hat{\mathcal{O}}$, following sum rule is valid.

$$[\hat{\pi}, \hat{\mathcal{O}}] = 0 \quad \text{or} \quad [\hat{\pi}, \hat{H}] = 0$$

$$\Rightarrow \quad \sum_{j\in\mathcal{X}} (E_j - E_i)|\langle i|\hat{\mathcal{O}}|j\rangle|^2 = \frac{1}{2}\langle i|[\hat{\mathcal{O}}, [\hat{H}, \hat{\mathcal{O}}]]|i\rangle, \quad \text{for} \quad {}^{\forall} i \in \mathcal{X}$$

Sum rule (Q_{20})

- Quadrupole operator

$$\hat{Q}_{20} := \sum_{n=1}^{A}(2\hat{z}_n^2 - \hat{x}_n^2 - \hat{y}_n^2)$$

$$\sum_{j\in\mathcal{X}}(E_j - E_i)|\langle i|\hat{Q}_{20}|j\rangle|^2 = \frac{2\hbar^2}{m}\left(1-\frac{1}{A}\right)\langle i|\sum_{n=1}^{A}(4\hat{z}_n^2+\hat{x}_n^2+\hat{y}_n^2)|i\rangle$$

kinetic + CoM (1-body)

$$-\frac{2\hbar^2}{mA}\langle i|\sum_{\substack{n,m=1\\ n\neq m}}^{A}(4\hat{z}_n\hat{z}_m+\hat{x}_n\hat{x}_m+\hat{y}_n\hat{y}_m)|i\rangle$$

CoM (2-body)

- GCM vs DGCM (left-hand side / right-hand side)

	$i = 1$ (ground state)	$i = 2$ (1st exited)	$i = 3$ (2nd exited)	$i = 4$ (3rd exited)	$i = 5$ (4th exited)
GCM	1.0005	0.6287	0.7309	0.6370	-0.5878
DGCM	1.0047	1.0162	1.0512	0.9414	0.6352

Better results for the DGCM

Why is the DGCM better?

- Why is the DGCM better?

Under several conditions, the constrained variational method + DGCM has the following structure,

$$\overline{\mathrm{Span}}(\{|q,p\rangle\}_{q,p}) = \mathcal{H}_C \otimes \mathcal{H}_{NC}^{\mathrm{sub}}$$

"collective subspace" = "collective part" $\otimes$ "non-collective part"

➡ $[\hat{\pi}, \hat{Q}_{20}] = 0$ (sum rule is satisfied)

It is expected that the separable structure could be obtained for the quadrupole oscillation.

Summary

■ Summary

- ✓ Separable structure of the collective subspace in the constrained variational method + DGCM
- ✓ Comparison of the GCM and the DGCM for the quadrupole vibration
- ✓ The DGCM can efficiently generate different basis functions
- ✓ The remarkable difference is observed in the sum rule for $\hat{Q}_{20}$

■ Future perspective

- ✓ Application to heavy nuclei such as ^{238}U
- ✓ Application to other deformation modes
- ✓ Classification of GCMs in terms of structures of manifolds.

Thank you for listening